REPORT DOCUMENTATION PAGE

Form Approved OMB NO. 0704-0188

1. REPORT DATE (DD-MM-YYYY)	2. REPORT TYPE	3. DATES COVERED (From - To)
07-12-2009	Final Report	1-Jul-2005 - 31-Aug-2009

4. TITLE AND SUBTITLE
Final Report for Project W911NF0510380 / 4700 MA

5a. CONTRACT NUMBER
W911NF-05-1-0380

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER
611102

5d. PROJECT NUMBER
611102

5e. TASK NUMBER

5f. WORK UNIT NUMBER

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8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
U.S. Army Research Office
P.O. Box 12211
Research Triangle Park, NC 27709-2211

10. SPONSOR/MONITOR'S ACRONYM(S)
ARO

11. SPONSOR/MONITOR'S REPORT NUMBER(S)
47004-CS.6

12. DISTRIBUTION AVAILABILITY STATEMENT
Approved for Public Release; Distribution Unlimited

13. SUPPLEMENTARY NOTES
The views, opinions and/or findings contained in this report are those of the author(s) and should not contrued as an official Department of the Army position, policy or decision, unless so designated by other documentation.

14. ABSTRACT
This report describes work done on the ARO funded project "Air/Water Flow in Porous Media: A Comparison of Accurate and Efficient Numerical Models". We have analyzed and implemented a variety of algorithms for simulation of porous media flow, for coupled free flow and porous media flow regions, where the fluid is non-Newtonian, and for convection-diffusion equations. Our work has been presented at various conferences and published in a range of refereed journals. We have worked closely with researchers at the

15. SUBJECT TERMS
air/water flow, numerical analysis, temporal integration methods

16. SECURITY CLASSIFICATION OF: a. REPORT	b. ABSTRACT	c. THIS PAGE	17. LIMITATION OF ABSTRACT	15. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
UU	UU	UU	UU		Eleanor Jenkins
					19b. TELEPHONE NUMBER
					864-656-6907

Scientific Progress for W911NF-05-1-0380
Air/Water Flow in Porous Media: A Comparison of Accurate and Efficient Numerical Methods

1 Introduction

The research funded under this grant focused on solution algorithms for porous media flow models. We sought to improve both spatial and temporal computational methods for a range of problems associated with groundwater and surface water flows.

Groundwater flow problems can be difficult to resolve for several reasons. The governing equations are nonlinear, as the permeability coefficient for the Darcy velocity depends on the saturation level. This dependence on saturation also means that the governing equation can change type, from parabolic to hyperbolic, or vice versa, as an infiltration front moves through the domain. In addition, the governing equation can change type as fluid flows from one material type to another (e.g., from sand to clay). In all cases, the challenges are both on the temporal and spatial domains.

2 Unsaturated Flow

Richards' Equation is still one of the dominant modeling equations for vadose zone flow. The equation can be formulated with either water pressure or water saturation as the primary unknown, or the equation can be posed in mixed form where both variables appear as unknowns. While modeling vadose zone behavior is increasingly simulated using two-phase flow equations, resolution of Richards' Equation remains popular because the size of the systems is significantly smaller than that for the two-phase equations. In addition, the two phase equations include model equations for a compressible fluid (i.e., air), which pose computational difficulties as the density of the fluid now depends on the air pressure.

Accurate solution of Richards' Equation requires resolution in both space and time. Both spatial and temporal adaptive routines have been studied for this problem, as have higher order discretization methods in both space and time. The state-of-the-art in adaptivity was pushed forward for Richards' Equation in [11]. In that article, Farthing and his co-authors designed a space-time error measure and algorithm for Richards' Equation. They base their algorithm on a loose coupling of the two distinct discretizations to enable users to take advantage of existing, mature spatial and temporal adaption technology. This approach is important for ARO applications as extensive effort has been invested in developing flow simulation codes. The loose coupling allows these codes to be reused with significant improvements in accuracy and efficiency.

The space/time adaptive algorithm was extended in [9], [10] to use local discontinuous Galerkin methods for spatial discretization. The discontinuous Galerkin method is attractive because of it ability to conserve mass locally, to increase the order of the approximation in specific regions of the domain, to accurately approximate solutions that are discontinuous or nearly discontinuous, and to parallelize easily. The primary drawback is that there are a large number of degrees of freedom associated with the discrete system. This difficulty is overcome by using discontinuous Galerkin methods only in subregions of the domain that benefit from their use, which is described and analyzed in [9], [10].

3 Heterogeneous Media

We developed a test set of real-word, physical application problems that would exhibit the numerical difficulties associated with their simulation. The set included problems from the literature and problems that are inherently ill-conditioned, yet scientifically important. The document included descriptions of:

- infiltration problems with increases in levels of the water table;
- trenches lined with relatively impermeable materials, much like landfills;
- flow throughly media with variably distributed heterogeneity.

Much of the work centered around resolution of Richards' Equation, but the techniques developed to handle problems in this test set can be extended to handle two-phase flow equations. The test set was uploaded and described in an interim progress report.

4 Coupled Free Flow and Darcy Flow

A significant amount of work has been done in the last decade to develop algorithms for resolving coupled Stokes and Darcy flows (see, for instance, [8] and references therein). However, this work has involved Newtonian fluids, where the extra stress tensor is directly proportional to the deformation tensor. The constant of proportionality is the dynamic viscosity of the fluid. We have examined this coupling for non-Newtonian fluids, where the viscosity of the fluid is non-constant and depends on the magnitude of the deformation tensor [7]

5 Resolving Coupled Parabolic/Hyperbolic Flow

We have also developed algorithms for simple post-processing of discrete, continuous Galerkin approximations of the convection-diffusion equations where the equation type changes in both space and time. Sharp fronts appear in the transition region as the equation moves from hyperbolic to parabolic, and numerical approximations along the front exhibit local, non-physical oscillations. Upwinding methods have been used to resolve this problem, as have discontinuous Galerkin and local discontinuous Galerkin methods. Upwinding methods often perform poorly when the grid is not aligned with the primary flow direction, and, in temporally dependent problems, the operator must be reconstructed at each time step. As mentioned earlier, discontinous Galerkin methods use large degrees of freedom, and local discontinuous Galerkin methods require remeshing in temporally dependent problems where the sharp front moves as a function of time (e.g., infiltration problems). In [6]

In this example, the domain is parabolic on $[0, 1)$, hyperbolic on $[1.5, 2)$, and parabolic again on $[2, 2.5]$. We define $t \in [0, 2]$, with $\Delta t = \frac{1}{128}$. The true solution is given by the function

$$u(x,t) = \begin{cases} -\sin(x-1) + \exp(x-1) + t(x-1)^2, & 0 \le x < 1 \\ (x-1)^2(t+1) - 1, & 1 \le x < 1.5 \\ 1 + (x-1.5)\left(x^2 + (0.25t - 3.5)\,x + (2.75 - 0.625t)\right), & 1.5 \le x \le 2 \end{cases}$$

The solution is discontinuous at 1.5, but the flux is continuous on $[0, 2]$. The unstabilized solution exhibits highly oscillatory behavior, but both of the stabilized solutions remove these oscillations.

The approximation is computed on a grid with $h = \frac{1}{32}$ and $\Delta t = \frac{1}{128}$. In the two grid solution, shown on the right in Figure 2, the smoothing operator is computed on a grid with $h = \frac{1}{64}$.

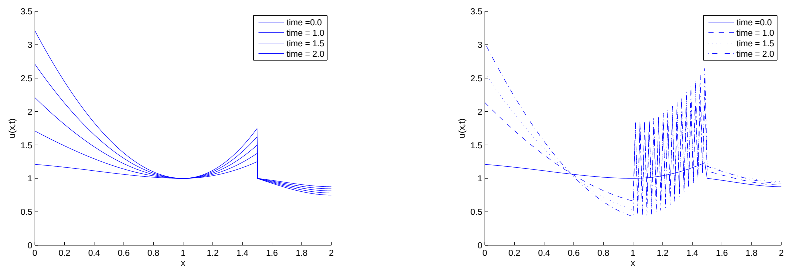

Figure 1: True solution (left), unstabilized solution (right)

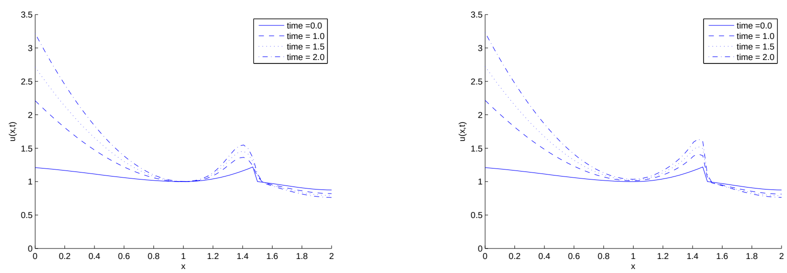

Figure 2: Smoothed solution on one grid (left) and two grids (right)

We have also applied the operator to one- and two-dimensional infiltration problems. The one-dimensional results are shown in Figures 3 and 4, and the two-dimensional results are in [6]. The one-dimensional problem shows the solution to the governing equation

$$u_t + uu_x - 0.001u_{xx} = f, \quad -1 < x < 4, \quad t > 0.$$

where f is defined so that the true solution is

$$u(x,t) = 1 - \tanh\left(\frac{1}{0.002}(x-t)\right).$$

The true solution is shown on the left in Figure 3, and the unstabilized solution is shown on the right.

The results on the left in Figure 4 were computed by solving the convection-diffusion operator and the filtering operator on the same grid. The results on the right were obtained by applying the filter operator on a grid with

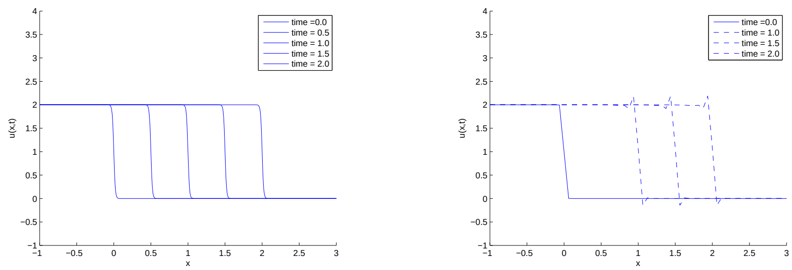

Figure 3: True solution (left), unstabilized solution (right)

twice the resolution of the solution grid. The results are enhanced by filtering on the finer grid because the goal of the filter is to resolve errors on the subgrid scale.

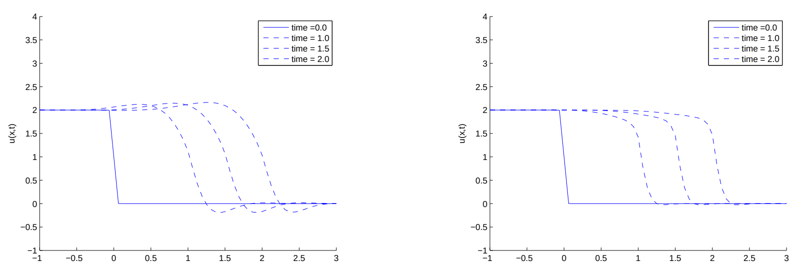

Figure 4: Smoothed solution on one grid (left) and two grids (right)

6 Temporal Integration for Non-Newtonian Flows

We have done a significant amount of work has been done to improve temporal integration for non-Newtonian flows. The modeling equations for non-Newtonian flows require resolution of the fluid's stress, velocity, and pressure. The conservation equations for mass and momentum represent a "Stokes-like" system, and the constitutive equation for stress is a hyperbolic partial differential equation. Instead of solving the entire coupled system implicitly, we computed using sub-steps of a given time step Δt. The conservation equations were resolved in the first fraction of the time step, using a lagged value for stress. These solutions were used in the next fraction of the step to update the stress, and the updated value for stress was used to compute a final velocity and pressure over the time step. This strategy allows one to apply stabilization techniques over a fraction of a time step instead of the entire time step, reducing the damping effects of added diffusion operators.

We began the research by focusing on the convection-diffusion equation. While operator splitting techniques have frequently been applied to this equation, our strategy differed in that we combined features of both additive decomposition algorithms (such as alternating direction implicit and implicit/explicit schemes) with product decomposition algorithms. The additive decomposition algorithms decompose the operator and treat variables either implicitly or explicitly at each fraction of the time step. Product decomposition algorithms advance the convective part of the operator first and use this to advance the diffusive part of the operator over the entire time step.

We obtained optimal a-priori estimates for our scheme for both the convection-diffusion equation and the equations for viscoelasticity. We showed the validity of the scheme for several applications problems, including a moving front problem, a rotating cone problem, and a contraction problem from the viscoelasticity literature. John Chrispell received his Ph.D. in 2008, under my supervision and that of Professor Vince Ervin. Dr. Chris Kees of the US Army ERDC served on his Ph.D. committee. John spent summers at ERDC and implemented his algorithm in PyADH, an ERDC research hydraulics code.

The work on this project was jointly funded by NSF under grant No. DMS-0410792 and this ARO grant. It is summarized in [3, 4, 5] and [2].

7 Computation of Navier-Stokes Equations

V.J. Ervin has worked on extending the enhanced-physics based scheme for three-dimensional Navier-Stokes equations [1]. The general enchanced physics based scheme (preserving helicity) for the NS equations introduced by Rebholz is based on expressing the NS equations in curl-form. In the curl-form the pressure term in the equations is the Bernoulli pressure $(p + 1/2|u|^2)$. Due to the behavior of $|u|^2$ in or near the boundary layers, the Bernoulli pressure term can contribute significant computational instability to the approximation. In [1]. Ervin, Rebholz, et.al. investigated and showed the positive effect of grad-div stabilization on the enhanced physics approximation scheme.

Ervin is also working in improvements to computational solutions of the Navier-Stokes equations using filtering. The scheme mirrors the scheme outlined in [6], in that the filtering operator acts as a post-processing operator for the solution to the discrete, unstabilized operator. There are theoretical results to show that the filtering scheme reduces the effects of high-frequency components that appear in the computed solution

The paper associated with this work will be submitted within the next six months.

8 Student Involvement

While student involvement does not directly connect with scientific progress, I wanted to add this section to discuss the impact that this funding has had on John Chrispell, who received a Ph.D. in mathematical sciences while being partially funded by ARO. John was able to spend two summers working with Dr. Chris Kees at the US Army ERDC in Vicksburg, MS. Chris is an expert in numerical methods for porous media flow, and he is well versed in a variety of software languages. John learned of physical applications for his work on convection-diffusion equations, he enhanced his computational skills, and he implemented his operator-splitting algorithm in a real-world simulation code. He worked in an interactive, laboratory environment and was able to learn from engineers whose daily work requires extensive knowledge of flow problems, resolution of computed solutions with underlying physical behavior, computational skills, and the ability to effectively communication through papers and presentations. It is impossible to underestimate the benefit he received from his work there. Students whose whole tenure is spent in the purely academic setting can never truly embrace the concept of "applied mathematics". I am extremely grateful to ARO for allowing me to provide this experience for my students.

References

[1] M.A. Case, V.J. Ervin, A. Linke, L.G. Rebholz, and N.E. Wilson. Stable computing with an enhanced physics based scheme for the 3d Navier-Stokes equations. submitted for review, 2009.

[2] J.C. Chrispell. *Numerical analysis of a fractional-step θ-method for fluid flow problems.* PhD thesis, Clemson University, 2008.

[3] J.C. Chrispell, V.J. Ervin, and E.W. Jenkins. A fractional step θ-method for convection-diffusion problems. *Journal of Mathematical Analysis and Applications*, 333:204–218, 2007.

[4] J.C. Chrispell, V.J. Ervin, and E.W. Jenkins. A fractional step θ-method for viscoelastic fluid flow using an SUPG approximation. *International Journal of Computational Science*, 2(3):336–351, 2008.

[5] J.C. Chrispell, V.J. Ervin, and E.W. Jenkins. A fractional step θ-method approximation of time-dependent viscoelastic fluid flow. *Journal of Computational and Applied Mathematics*, 232(2):159–175, 2009.

[6] V.J. Ervin and E.W. Jenkins. Stabilized approximation to time dependent conservation equations via filtering, 2009. submitted for review.

[7] V.J. Ervin, E.W. Jenkins, and S. Sun. Coupled generalized nonlinear Stokes flow with flow through a porous medium. *SIAM Journal on Numerical Analysis*, 47(2):929–952, 2009.

[8] V. Girault and B. Rivière. DG approximation of coupled Navier-Stokes and Darcy equations by Beaver-Joseph-Saffman interface condition. *SIAM Journal on Numerical Analysis*, 46:2052–2089, 2009.

[9] H. Li, M.W. Farthing, C.N. Dawson, and C.T. Miller. Local discontinuous Galerkin approximations to Richards' Equation. *Advances in Water Resources*, 30(3):555–575, 2007.

[10] H. Li, M.W. Farthing, and C.T. Miller. Adaptive local discontinuous Galerkin approximation to Richards' Equation. *Advances in Water Resources*, 30(9):1883–1901, 2007.

[11] Cass T. Miller, Chandra Abhishek, and Matthew W. Farthing. A spatially and temporally adaptive solution of Richards' Equation. *Advances in Water Resources*, 29(4):525–545, 2006.